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Title:	Eulerian Applications Project - xRage Introduction and Overview
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Eulerian Applications Project - xRage

Introduction and Overview

EAP

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NNSA
National Nuclear Security Administration

WHAT IS XRAGE?

Overview

I. History
II. Supported Physics
III. Eulerian Methods
IV. Adaptive Mesh Refinement
V. Example Applications

History of xRage

- Rage is an acronym of "Radiation Adaptive Grid Eulerian"
- xRage is the name adopted by LANL when it took control of the code in the mid 2000's
- The code was originally developed by Science Applications International Corporation (SAIC)
  - Lead Developer – Michael Gittings
    - Additional support was provided by a team of SAIC employees and contractors
- Originally the code was named SAGE for Saic Adaptive Grid Eulerian
  - Cray Fortran 77 code intended for the current supercomputing environment in the 1980s and early 1990s (aka Cray I/XMP/YMP/2)
  - Highly vectorized for performance
  - Applications included seismic waves in rock
- In the middle 1990s a collaboration was initiated between Gittings and laboratory scientist Robert Weaver during a sabbatical Weaver took to visit SAIC in San Diego
  - This collaboration led to the addition of radiation diffusion into the code and its adoption by Los Alamos as a research code

History of xRage

- In the mid 1990s Gittings moved to Los Alamos to serve as the chief developer of Rage at Los Alamos
  - Additional developers from LANL, mainly from X-Division, were also added to the project
  - Additional personnel from SAIC also participated in the LANL contract to support Rage
- Rage provided significant new capabilities for the hydrodynamic simulations with its adaptive mesh capabilities
  - Early successes include simulations of the shock curtain experiments of Robert Benjamin and Kathy Prestridge
- With the introduction of new Fortran standard the source code of Rage was converted to Fortran 90
  - This software port was important in the transition from the original Cray family of computers to the minicomputer environment that was to displace Cray as the platform of choice for scientific computing.

History of xRage

- In the early 2000s the DOE introduced the Advanced Simulation and Computing Initiative (ASCI) and Rage was adopted by LANL as one of its original ASCI codes
  – This promotion of Rage from a research code to an ASCI code led to the expansion of LANL development team
- In the mid 2000’s the core hydrodynamic method for Rage was converted from a Lagrange plus remap method to a finite volume Godunov inspired scheme
  – This so-called Cruise version was developed by Gittings while he was on a round-the-world cruise
- The new capabilities provided by the Godunov based hydro scheme were significant improvements in the simulation capabilities.

History of xRage

- By this time LANL had been fully funding the Rage development project for a decade and management felt that it was time for Los Alamos to assume full control of the code base.

The birth of xRage

- Since the transition many new capabilities and features for both research and user requests have been added. Subsequent lectures will highlight many of these features and describe their basic usage.
- More recently much of the development of this code has focused on software organization and the use of external libraries. These features are of great interest to developers but may not generally impact users.
- The biggest impact on users has been the enhancement of the ability of the code to run at scale for very large problems. The EAP logo shown on the title page was taken from a large scale 3D simulation of the high velocity impact of a comet.

Warning: xRage is an Export Controlled Code

- The source code for xRage is export controlled and distribution of this source without proper authorization is asking for trouble (i.e. illegal)
- DON'T SHARE THE SOURCE! Collaborators who wish access to this code should request it through proper laboratory channels
  - Visit: https://asc.lanl.gov to initiate a request for access to the source code for xRage
    - The request requires management approval and justification
- Once access is granted you wish to obtain access to the EAP confluence space on https://xcp-confluence.lanl.gov/.
    - This site contains many useful tips on the code and its usage.
- Developers will generally also require checkout and commit privileges and gitlab access on https://xcp-gitlab.lanl.gov/
- Details on how to checkout the code are available on the EAP confluence space
    - An email to crestone_support@lanl.gov will usually get you in touch will someone who can help with these issues.
- Generally users may run release executables of this code without the export control restrictions that apply to the source code. Compiled releases can be found on the HPC platforms at /usr/projects/eap/releases with the most current releases in the directory latest.
  - Access requires membership in the Unix group dacodes which will be granted by the software request mentioned above.

What can xRage Do?

- xRage is a Multi-Material/Multi-Physics/Adaptive-Mesh-Refinement Eulerian code
  - Eulerian in this context means the flow state is solved on a spatially fixed mesh (more specifically, the mesh does not change during a time step cycle)
  - Adaptive mesh refinement means that after a time step cycle, the mesh can be modified to add/remove computational cells based on the current flow state.
- The code supports solutions in one dimensional spherical or cylindrical geometry, two dimension axi-symmetric geometry, and one, two, and three dimensional rectangular geometry
- This basic code has options to model
  - Compressible Hydrodynamics
  - High explosives
  - Material Strength (elastic/plastic flow)
  - Radiation diffusion
  - Laser Physics
  - Plasmas
  - Turbulence (via Reynolds Averaged Navier-Stokes formulations)

Basic Eulerian Hydrodynamics

- xRage solves the compressible Euler equations that describe the conservation of mass/momentum/energy

$$\frac{\partial \rho \mu_k}{\partial t} + \frac{\partial \rho \mu_k u_j}{\partial x_j} = 0$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial P}{\partial x_i} = 0$$

$$\frac{\partial \rho \left[\frac{1}{2}u^2 + e\right]}{\partial t} + \frac{\partial \rho u_j \left[\frac{1}{2}u^2 + e\right]}{\partial x_j} + \frac{\partial P u_j}{\partial x_j} = 0$$

- Here ρ is the mass density, $\mathbf{u} = \{u_i\}$ is the flow velocity, P is the thermodynamic pressure, and e is the specific internal energy. The quantities μ_k are the mass fractions of the material components in the flow.
- The system is closed by the equations of state for the material components via the Amagat, or pressure-temperature equilibrium condition

$$1/\rho = V = \sum_{k=1}^{N} \mu_k V_k(P,T), e = \sum_{k=1}^{N} \mu_k e_k(P,T)$$

- The above system is solved for the pressure and temperature given the total density, specific internal energy, mass fractions, and equations of state for the separate material components.

Discretization of the Euler Equations

- Numerical solutions of partial differential equations require the flow equations be cast into an approximate discrete form suitable for solution on computers
- There is long history of approaches for solving such systems, dating back to the 1950's and earlier. The oldest approaches were based on finite difference approximations where the solution was represented as values on a discrete mesh and the partial derivatives were replaced by finite differences. A full description of the history of finite difference methods is beyond the scope of this course. Some highlights include:
  - Mid 1950 von Neumann artificial viscosity to improve shock resolution
  - Mid 1960s Second Order Lax-Wendroff method
  - Latter 20th century – very high order methods based on compact schemes
- There are too many other approaches to describe here. None of these are used as the default solver in xRage, although some may be present in developmental form.
  - A subsequent lecture will provide details on the default hydrodynamic solver.

Finite Volume Schemes

- The solver in xRage is based on the finite volume formulation. These methods generally apply to any system in divergence form
$$\frac{\partial U}{\partial t} + \nabla \cdot F = 0$$
- The vector $U(x,t)$ is usually called the state vector and the vector $F(x,t)$ is called the state flux or simply the flux. Most commonly the flux depends on space and time indirectly with the flux given as a function of the state $F(x,t) = F\big(U(x,t)\big)$.
- In our case we are only interested in hyperbolic systems, which means that the quantity $n \cdot \frac{\partial F}{\partial U}$ has all real eigenvalues for every spatial direction n.

Finite Volume Schemes

- The conservation equations from the previous slide are discretized over a fixed mesh by integrating the conservation equation over the space-time cell to yield the equation

$$U^{n+1} = U^n - \frac{\Delta t \, area(\partial\Omega)}{vol(\Omega)} F^{n+\frac{1}{2}}$$

$$U^n = \frac{1}{vol(\Omega)} \int_\Omega U(x, t^n) dV$$

$$F^{n+\frac{1}{2}} = \frac{1}{\Delta t \, area(\partial\Omega)} \int_{t^n}^{t^{n+1}} \oint_{\partial\Omega} F \cdot n dA$$

- In one space dimension the update over the interval $x_{i-\frac{1}{2}} \leq \mathrm{x} \leq x_{i+\frac{1}{2}}$ becomes

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x_i}\left(F_{i+\frac{1}{2}}^{n+\frac{1}{2}} - F_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right)$$

- The above formulas are exact, they become numerical by approximating the flux integrals.

Godunov Methods

- In 1959 Sergei K. Godunov proposed a finite volume scheme based on solutions to one dimensional Riemann problems
  - A Riemann problem is an initial value problem for a hyperbolic system with scale invariant initial data. In one space dimension this is an initial value problem with two constant states to the left and right of a discontinuity point
- The method is based on the finite volume formulation where the solution is piecewise constant on a fixed mesh, these constant values approximate cell averages for the “true” solution. Riemann problems are solved using the constant data on either side of a cell edge and the numerical flux is evaluated as the flux value computed from the Riemann problem solution at the cell edge.
- I won’t go into detail on all of the theory here, sufficient it to say there is a large body of books and articles on this topic.
- This basic idea is the Granddaddy of a great variety of numerical methods for solving hyperbolic systems, including xRage.

Higher Order Godunov Schemes

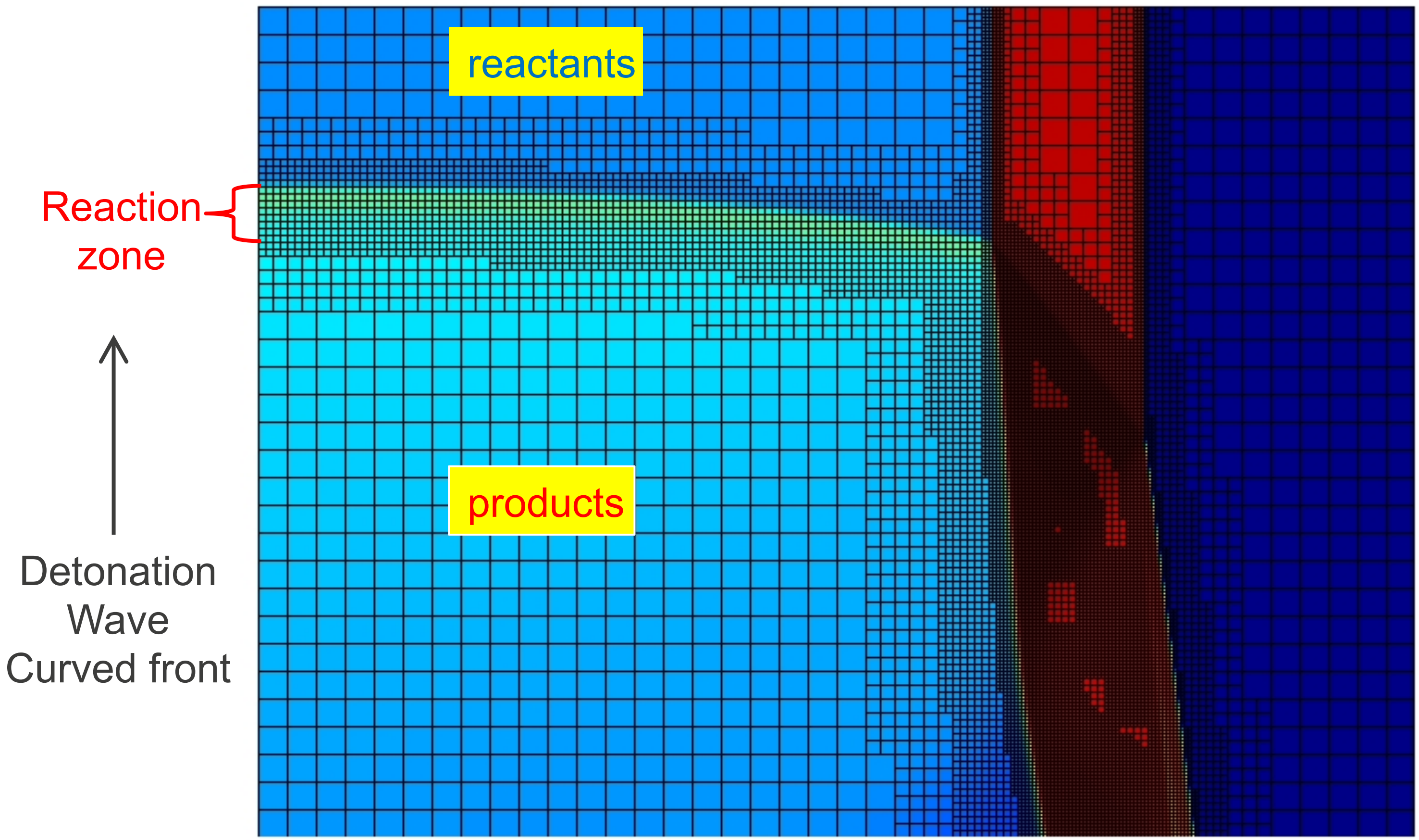
- While a very effective numerical scheme, in many cases, the basic Godunov scheme is only first order accurate and is too diffusive for many applications.
- In the 1970's Bram van Leer wrote a series of influential papers describing extensions of the basic Godunov method that provided higher order accurate approximations to solutions for hyperbolic conservation equations.
- The basic idea was to reconstruct spatially variable approximations to the flow state in a cell that preserved the cell average data given by the numerical approximation of the flow state.
  - Originally these were linear reconstructions.
  - Later higher order approximations (such as quadratic) were developed.
- Fluxes were computed using Riemann problem solutions with data taken by left and right edge values of the reconstructed fields.
- To prevent numerical oscillations in the solution slope limiting was applied to the reconstructed solution to eliminate the generation of new local extrema.
- Ahigher order Godunov scheme is the basic flow solver now in use in xRage (details will be provided in a subsequent lecture).

Continuous Adaptive Mesh Refinement

- The solution grid used in xRage is based on a binary-by-direction refinement grid.
- The grid is built from a basic square lattice (xRage only supports square cells).
- Each cell may be subdivided into 2^dsubcells by dividing the edges of the cell by 2.
- Continuous refers to the restriction that adjacent cells my not differ by more than one level of refinement, i.e. a cell may have at most two neighboring cells on any given side.
- The AMR used in xRage is a special case of block based AMR with a block size of two per direction.

AMR example, cylinder test simulation

Density plot with grid lines

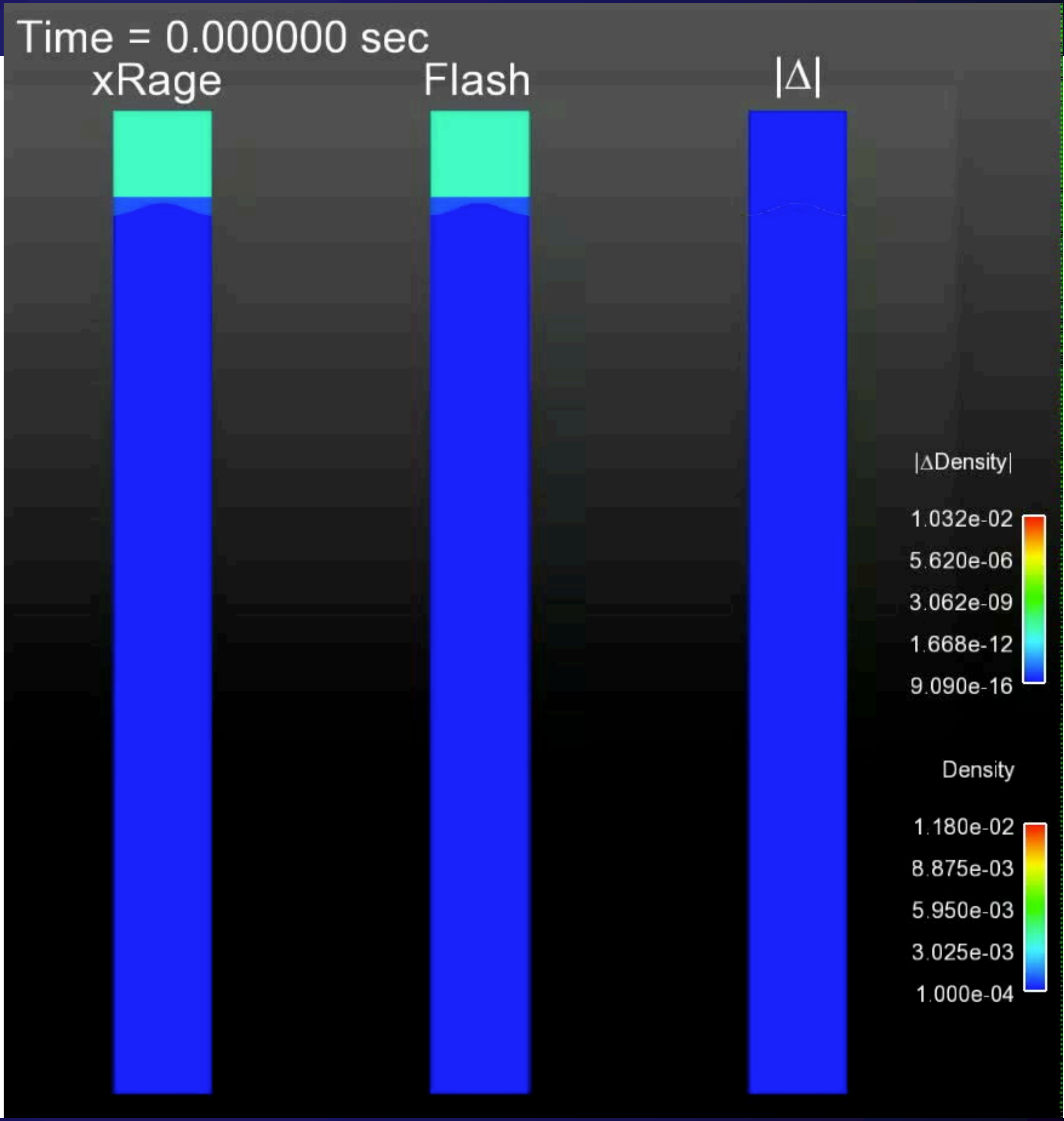


Examples

- The following slides show only a few of the types of problems that can be simulated by xRage
- This list is so far from exhaustive as to be ridiculous.
- The examples are just intended to give you a flavor of what the code can do.

Examples: Planar Richtmyer-Meshkov Instability

- Air to Helium refraction
  - 10 bar shock collides with an air/helium interface
- Comparison of xRage with the Flash hydrocode



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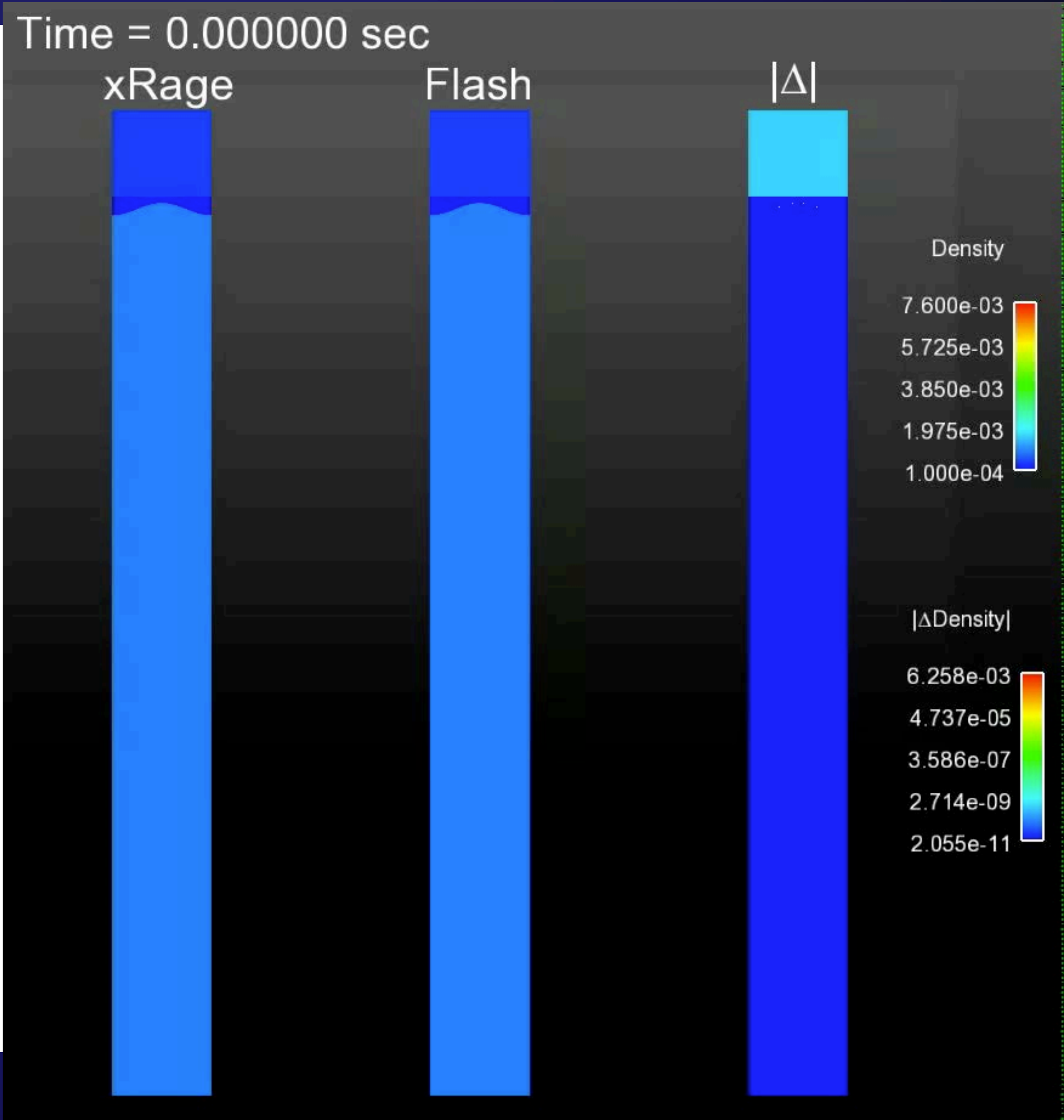
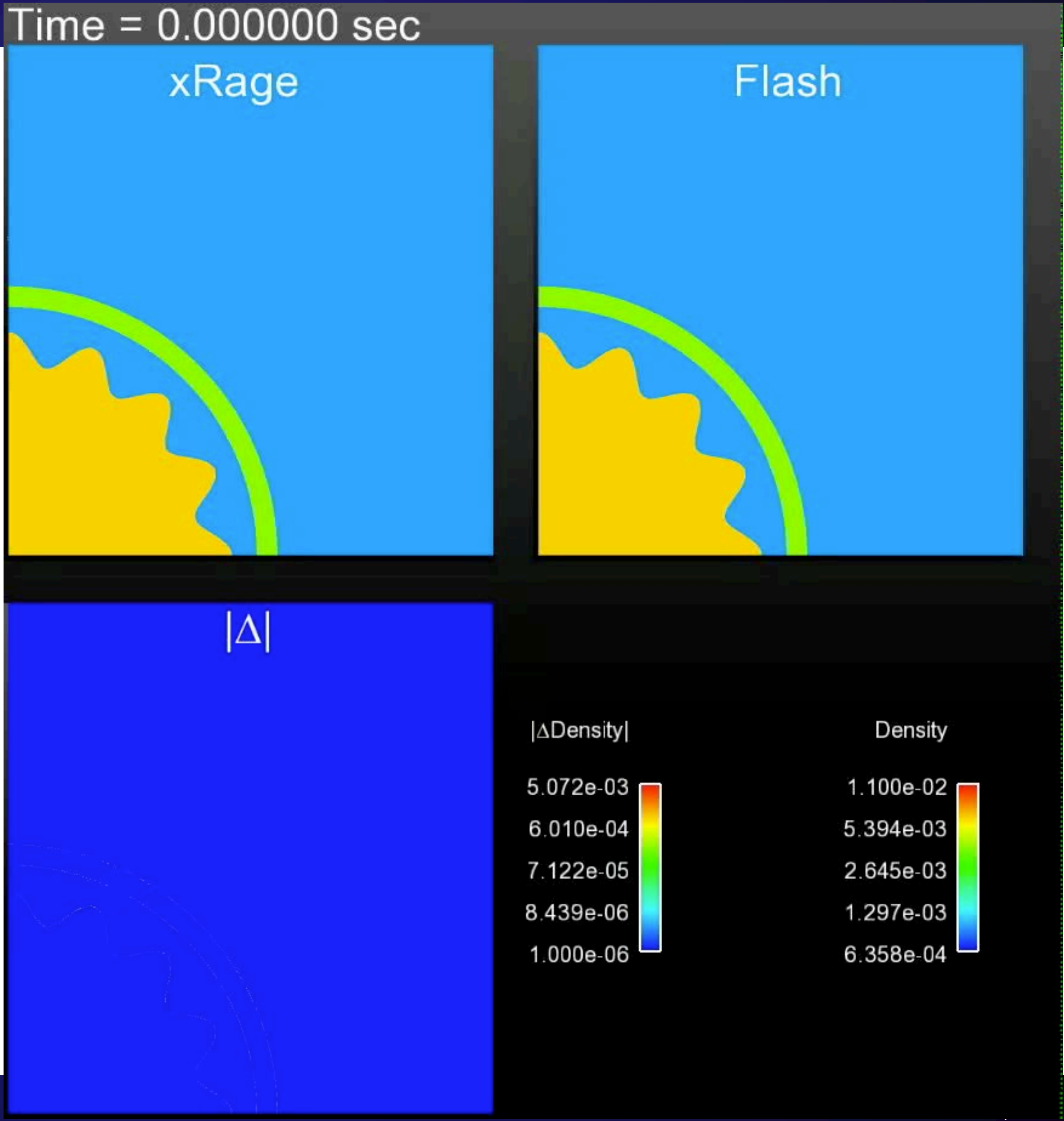


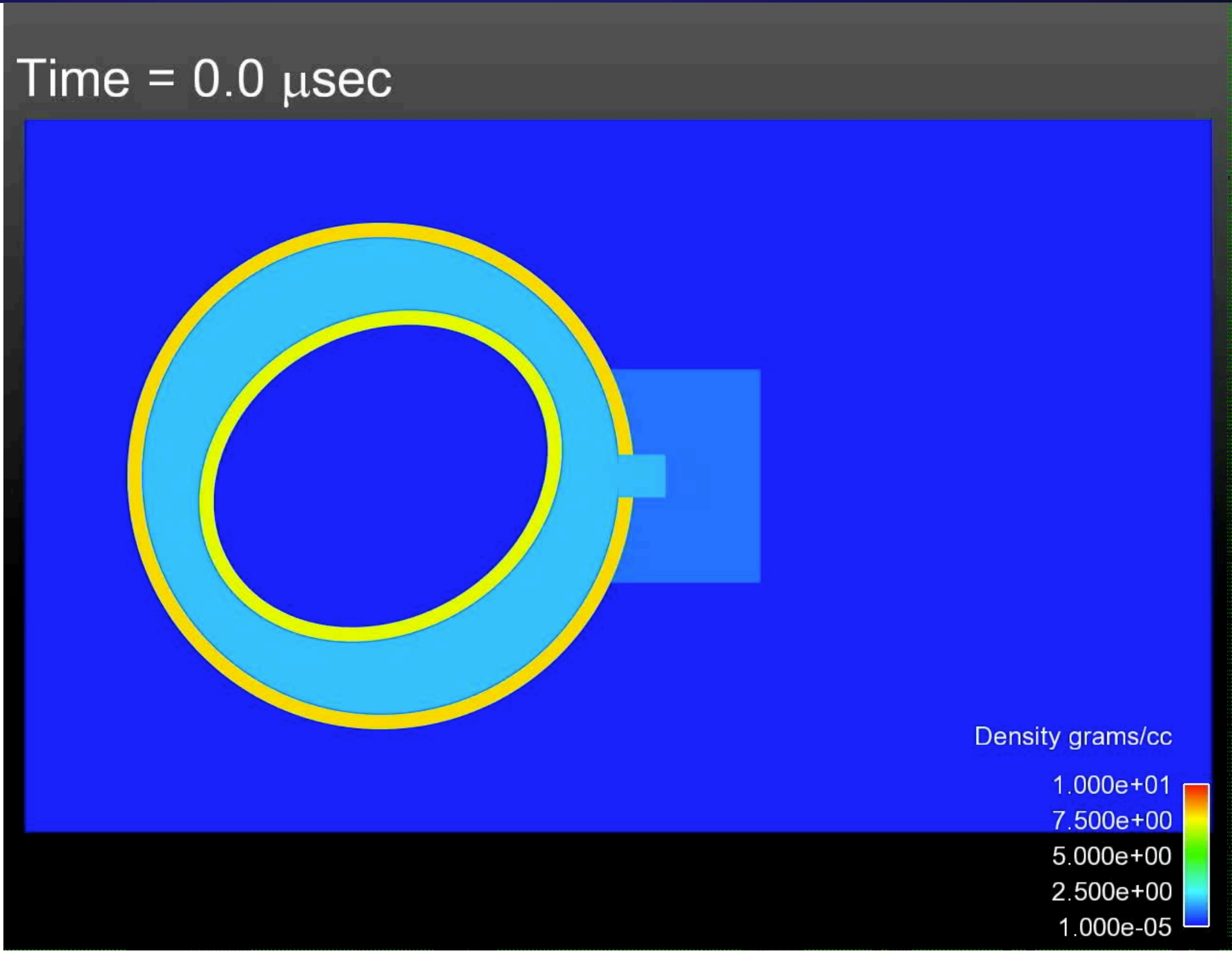
Imploding Richtmyer-Meshkov Instability

- Imploding shock from air into Sulphur-hexafloride



High Explosive Experiment

- Simulation of an experiment for propagating high explosive waves in PBX-90502



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